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6. AUTHOR(S)
Dr. David Kanis

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Chicago State University
Office of Sponsored Programs
9501 S. King Drive
Chicago, IL 60628

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Dr. Charles Y.-C. Lee
AFOSR/NL
110 Duncan Avenue Room B115
Bolling AFB DC 20332-8050

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13. ABSTRACT ***(Maximum 200 Words)***

The goal of this year-long research effort was to determine if we could streamline our Nonlinear Optical response computations by using commercially available software rather than the software developed in our laboratory. If our research efforts in this direction are to continue, the user-interfaces of our software must be within the capabilities of undergraduate researchers. Specifically we compared computed λ_{max} values with experimental values for over 400 dyes found in *The Sigma-Aldrich Handbook of Stains, Dyes, and Indicators*. We found that the user-friendly CAChe package is not a viable option in the evaluation of NLO responses, however, the more rigorous Cerius package does provide more reasonable responses relative to experiment. We believe that the most important factor in computing either an NLO response or a λ_{max} for these dye molecules is the ability of a given computational model to accurately determine the molecular geometry of these highly conjugated molecules.

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Air Force Office of Scientific Research

Final Report - for Grant F49620-97-1-0424

Computational Studies of Novel Nonlinear Optical Chromophores

Principal Investigator

David R. Kanis

Department of Chemistry and Physics
Chicago State University
9501 South King Drive
Chicago, IL 60628

I. Objectives:

The primary goals of this research effort was to establish an advanced computational chemistry facility at an urban institution and to involve undergraduate researchers in a meaningful research experience in computing the nonlinear optical responses for novel chromophores.

II. Summary of Accomplishments:

Research Facility.

This research grant in conjunction with two other research grants provided funding for us to purchase four servers, eight PC/MAC computers, two laser printers, and networking equipment for our laboratory. These grants also enabled us to purchase a number of contemporary computational chemistry software packages such as Gaussian, Cerius, Spartan, and CAChe for use by our undergraduates.

Participation of Undergraduates in Research Efforts.

Fifteen research students (all African-Americans) participated in our research effort, with four of them working on this particular research project at some point during their research experience. In addition three high school students participated in our research efforts for two summers. All students were trained on various software applications in our research efforts. The students that participated in this research project are listed below along with their current status:

Tiffany Burgess-Brown. Graduated from Chicago State University, presently working for Abbott Laboratories in North Chicago. Tiffany made two presentations on her work.

Howard Gholston. Graduated from Chicago State University, presently a graduate student in Materials Science at Northwestern University in Evanston.

Brian Clay. Graduated from Chicago State University, presently working for a chemical consulting company in Chicago.

Luckner Jean. Graduated from the Illinois Institute of Technology with an engineering degree. Will be attending graduate school next year.

Felicia Duran (High School Student). Currently in college.
Leo Crockett (High School Student). Currently in college.
Theresa Zuniga (High School Student). Currently in college.

Summary of Research Findings.

One of our goals in this year-long research effort was to determine if we could streamline our Nonlinear Optical response computations by using commercially available software rather than the software developed in our laboratory. If our research efforts in this direction are to continue, the user-interfaces of our software must be within the capabilities of undergraduate researchers. As detailed below, we found that the user-friendly Spartan and CAChe packages are not viable options in the evaluation of NLO responses, however, the more rigorous Cerius package does provide reasonable responses relative to experiment. We should note that the Cerius package is actually a commercially-available replica of our in-house algorithms. However, this package is much more demanding to use and beyond the typical undergraduate's abilities.

III. Details/Results of Research Efforts:

Motivation of Research Studies.

For the past decade many researchers in the field of nonlinear optical materials have come to realize that computational chemistry plays a crucial role in the selection of molecular chromophores to insert into high-efficiency frequency doubling materials. Mark Ratner, Tobin Marks and I published a study in 1993 in which the hyperpolarizability generated via a semiempirical sum-over-states approach computed for over 200 molecular units was compared with experimental EFISH values as shown in Figure I. Most of these chromophores possessed the signature donor-acceptor π-architectures, and the structures chosen for this study were the sum total of all the molecules for which EFISH experiments had been performed. The molecular geometries for each chromophore were carefully chosen, but not optimized via a semiempirical methodology. The results of this experiment were surprisingly satisfying as seen in Figure I.

Unfortunately, this method was tedious and time consuming. In one portion of this research we looked at the possibility of using molecular geometries optimized with MOPAC in our ZINDO-SOS studies. To test this possibility, we compared the computed λ_{max} with experimental λ_{max} for over 400 dye molecules. These conventional dye molecules were taken from *The Sigma-Aldrich Handbook of Stains, Dyes, and Indicators*. Researchers have long recognized the link between the absorption energy and the NLO response through the two-level model. We propose that if our computational prescription correctly reproduces the electronic transitions it will also provide hyperpolarizability values that will compare favorably with experiment.

Details of Calculations.

All CAChe studies followed a standard prescription available in CAChe software. Specifically the optimized molecular geometries were determined through an AM1 optimization. The absorption spectra were then computed with a ZINDO calculation involving configuration interaction of 100 transitions between filled and unfilled molecular orbitals. Simplistic computations including solvents in the calculations were carried out using the solvent option in the CAChe software, with the diameter of the cavity taken as the size of the molecule. Additional solvent computations were carried out by systematically altering the size of the solvent cavity, however, the qualitative results of these studies were not different from the studies taking the molecular size as the cavity diameter. Exploratory Spartan calculations and Cerius calculations were carried out in a similar manner.

Results of the Research Studies

The numerical results of the λ_{max} computations are reported in Appendix I. Note that in this chart we are comparing gas-phase calculations with solvent-phase experimental data. We are obviously not looking for absolute accuracy, rather a relative correlation between computed and experimental data. Note that this is a similar assumption made in most nonlinear optical computations that have appeared in the literature.

A graphical summation of the data (over 400 data points) listed in Appendix I is displayed in Figure II. Clearly there is little correlation between the computed λ_{max} and the experimental λ_{max}. Moreover, if we separate out results for chromophores in a given solvent, we also see little correlation between the computed and experimental results. In Figure III the computed λ_{max}

values for molecules measured in ethanol (14 data points) is presented, and there is a slight correlation between theory and experiment, however, the data shown in Figure IV contains the graphical results for chromophores in water (over 100 data points) and a correlation is not readily apparent. From this study we conclude that a systematic prescription for computing electronic state information necessary for NLO computations using the CAChe package is not an appropriate prescription despite its ease of use for undergraduate researchers.

We attempted to improve these results by including solvent corrections into the computation. These results did not yield significantly different results. We also used performed a serious of Spartan calculations, however the results were similar. We are currently looking at Cerius computations where we use a more sophisticated molecular geometry optimization routine (more costly) and the results for both λ_{max} and for β appear to be much improved. These computations are more sophisticated, and and we are presently trying to simplify these computations further so a large number of potential chromophores can be systematically evaluated for NLO activity.

IV. Personnel Associated with the Project

Project Participant	*Status*	
David R. Kanis	Faculty	CSU
Luckner Jean	Undergraduate Student	CSU
Brian Clay	Undergraduate Student	CSU
Howard Gholston	Undergraduate Student	CSU
Tiffany Burgess-Brown	Undergraduate Student	CSU
Felicia Duran	High School Student	
Leo Crockett	High School Student	
Theresa Zuniga	High School Student	

V. Published/Submitted Papers from this Grant

None. However we do anticipate the submission of a manuscript describing this research effort following the completion of our Cerius studies.

VI. Interactions/Transitions involving this research grant

Presentations at Meetings/ Invited Seminars:

Kanis *Board of Governors Science Conference, Chicago, IL
*Alliance for Minority Participation Research Conference, Chicago, IL
Illinois Institute of Technology, Chicago, IL

*Students presented research results from this grant at these meetings.

Transitions:

None

VII. Patents

None

IX. Honors/Awards

Kanis	Chicago State University Faculty Excellence Award	1997
Kanis	Chicago State University Faculty Excellence Award	1998
Kanis	Selection into Project Kaleidoscope's Faculty for the 21st Century	1997
Kanis	Received a CAREER grant from the National Science Foundation	1996

Figure 1

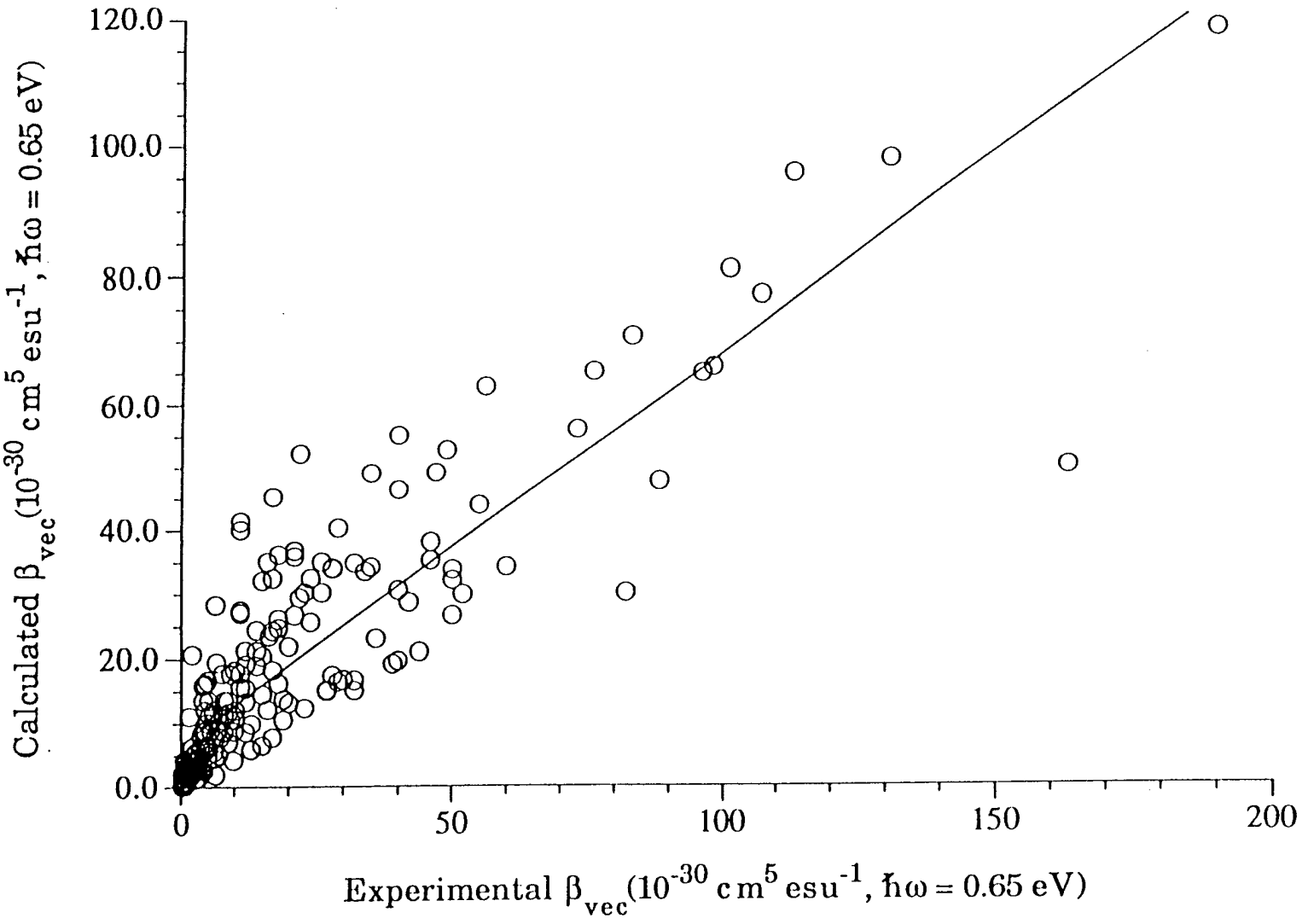

120.0
100.0
80.0
60.0
40.0
20.0
0.0
0
50
100
150
200
Calculated β_{vec} (10^{-30} c m^5 esu^{-1}, $\hbar\omega$ = 0.65 eV)
Experimental β_{vec} (10^{-30} c m^5 esu^{-1}, $\hbar\omega$ = 0.65 eV)

Figure 2

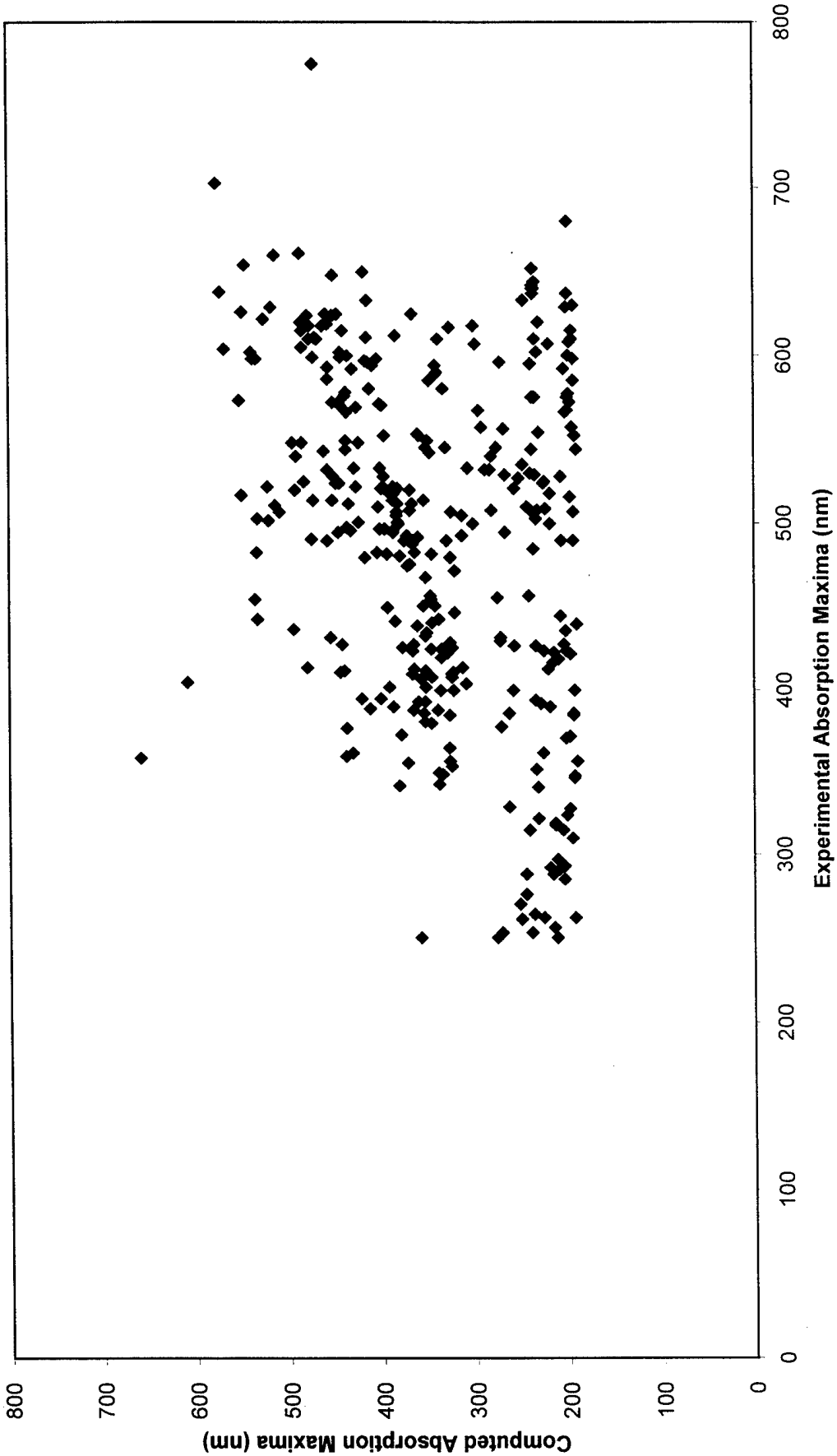

Computed Absorption Maxima vs.
Experimental Absorption Maxima for all Chromophores
Computed Absorption Maxima (nm)
Experimental Absorption Maxima (nm)
0
100
200
300
400
500
600
700
800

Figure 3

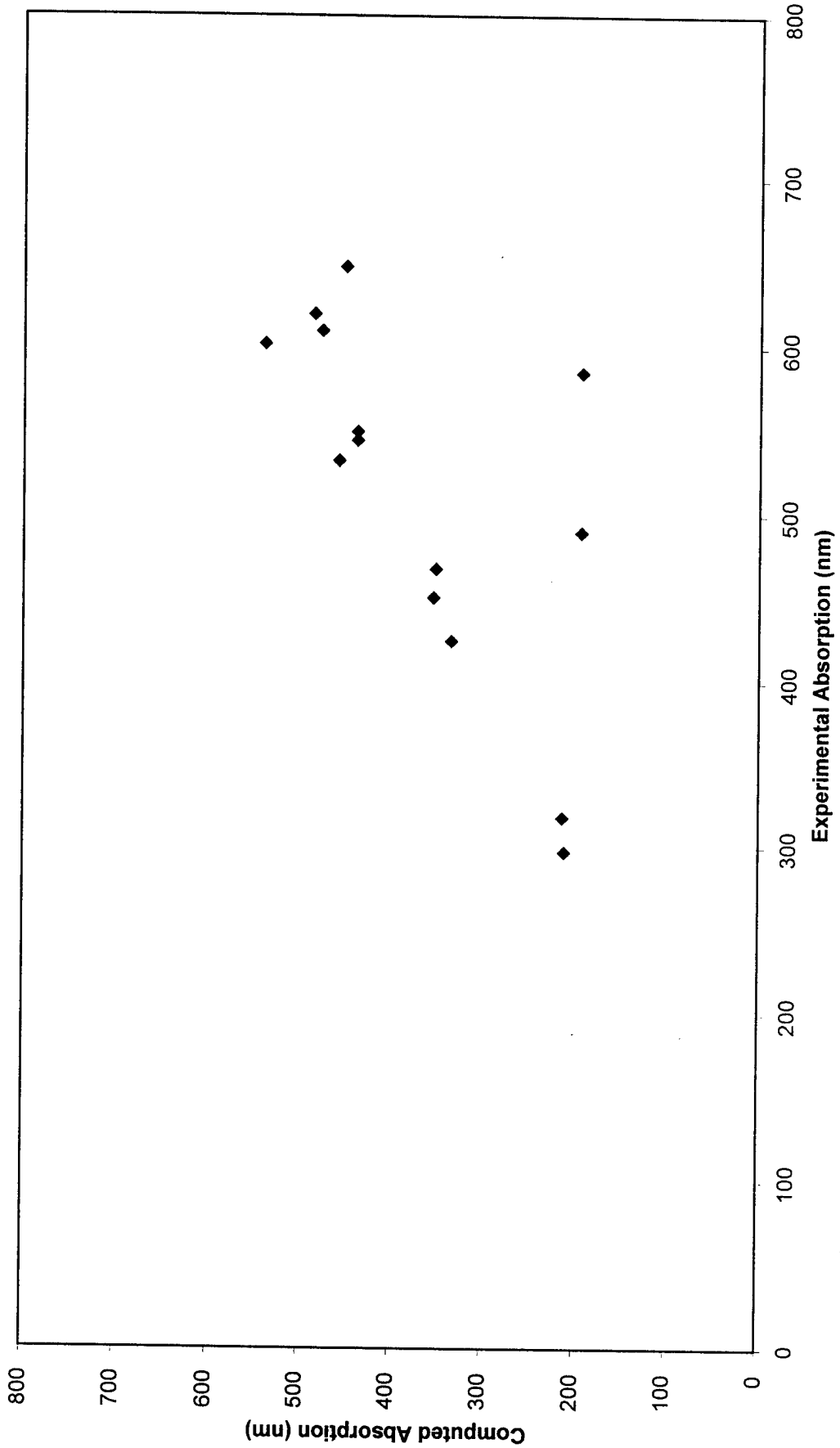
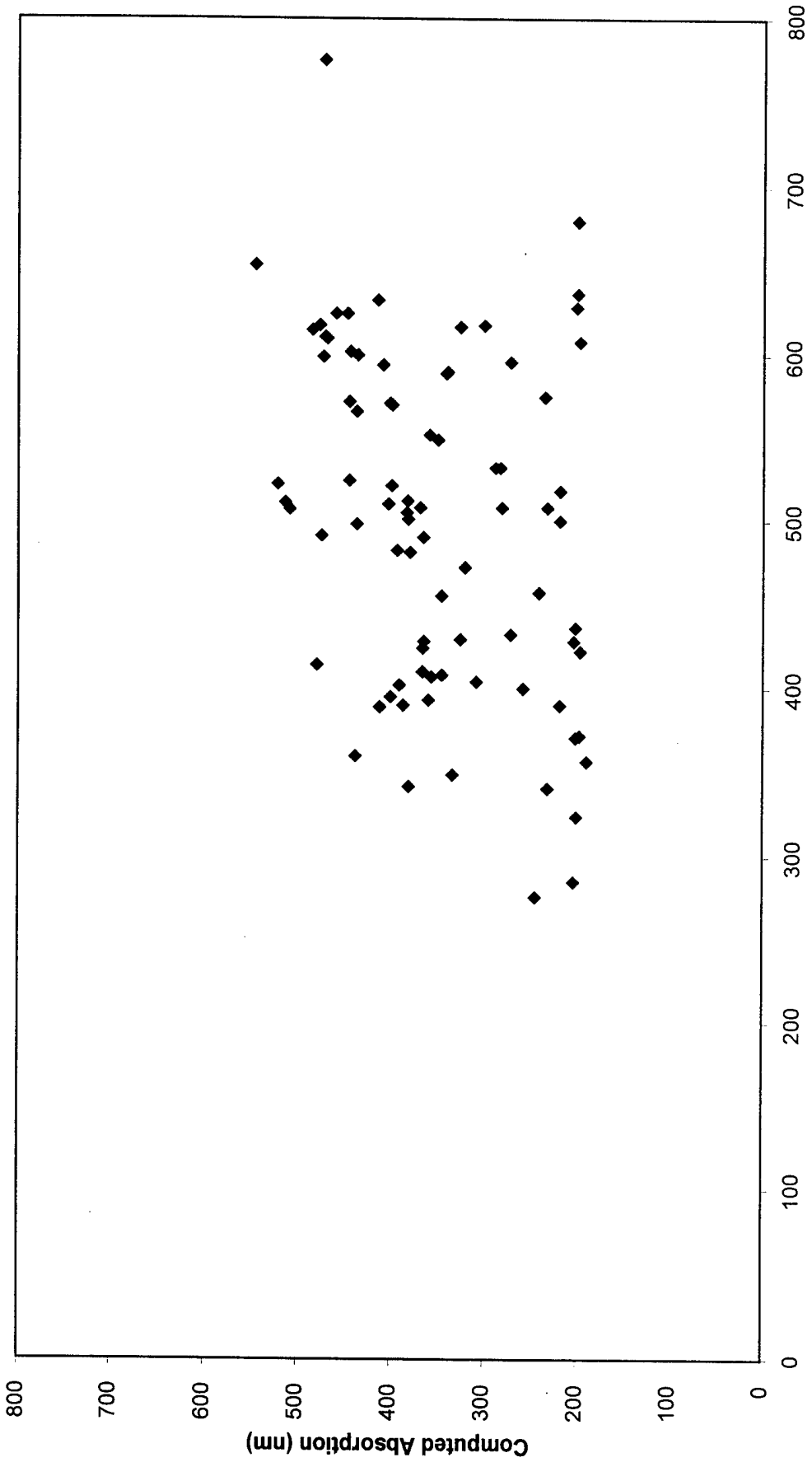

Computed Absorption Maxima vs.
Experimental Maxima for Molecules in Ethanol
Computed Absorption (nm)
Experimental Absorption (nm)
0
100
200
300
400
500
600
700
800

Figure 4


Computed Absorption Maxima vs.
Experimental Maxima for Molecules in Water
Computed Absorption (nm)
Experimental Absorption (nm)
0
100
200
300
400
500
600
700
800

Appendix 1

List of Dyes Examined from
The Sigma-Aldrich Handbook of Dyes, Stains, and Indicators

Appendix contains data for the CAChe generated Absorption Maxima for 363 Dyes. The Experimental data came from the Handbook, the Computed data came from performing a MOPAC geometry optimization on the molecule followed by a ZINDO computation of λmax.

Dye	#	EXP Abs. (nm)	Solvent	Computed Abs. (nm)
Acid Alizarin Violet N	1	501	Water	381.93
Acid Black 24	2	572	Water	444.94
Acid Blue 25	4	600	Water	435.96
Acid Blue 29	5	602	Water	443.69
Acid Blue 40	6	610	Water	468.74
Acid Blue 41	7	599	Water	472.99
Acid Blue 80	10	625	Water	459.17
Acid Blue 92	11	571	Water	401.35
Acid Blue 113	13	566	Water	436.98
Acid Blue 120	15	524	Water	444.99
Acid Blue 129	17	629	Water	201.53
Acid Green 41	24	680	Water	200.33
Acid Orange 8	25	490	Water	365.61
Acid Orange 63	27	424	Water	366.20
Acid Orange 74	28	455	Water	346.13
Acid Red 1	29	532	Water	288.24
Acid Red 4	31	508	Water	281.31
Acid Red 8	32	508	Water	232.59
Acid Red 88	35	505	Water	383.32
Acid Red 97	36	498	Water	436.85
Acid Red 106	37	532	Water	283.05
Acid Red 114	38	514	50% Ethanol	387.10
Acid Red 151	39	512	Water	382.52
Acid Yellow 34	50	408	Water	345.41
Acid Yellow 40	52	412	Methanol	352.12
Acid Yellow 42	53	410	Water	366.41
Acid Yellow 65	54	414	Water	479.49
Acid Yellow 76	55	393	50% Ethanol	352.51
Alcian Yellow	73	388	Methanol	365.35
Alizarin	75	567	0.1 N NaOH	200.49
Alizarin Complexone dihydrate	78	427	Methanol	234.18
Alizarin Red S monohydrate	80	556	0.1 N NaOH	268.32
Alizarin Violet 3R	82	540	Methanol	281.67
Alizarin Yellow GG	84	362	Methanol	430.48
Alphazurine A	87	637	Water	200.49
Aluminon	90	542	0.1N NaOH	347.47
Amaranth	92	521	Water	399.59
9-Aminoacridine hydrochloride monohydrate	94	400	Water	258.28
Astrazon Orange G	102	490	Methanol	207.00

Dye	#	EXP Abs. (nm)	Solvent	Computed Abs. (nm)
Auramine O	103	432	Water	271.79
Aurintricarboxylic Acid	105	545	0.1 N NaOH	330.51
Aurintricarboxylic Acid, Trisodium Salt	106	545	0.1 N NaOH	351.92
Azure A	109	633	Water	414.38
Azure B	112	648	Ethanol	451.28
Basic Blue 3	123	654	Water	546.00
Basic Blue 47	124	610	Methanol	235.00
Basic Blue 66	125	615	Water	485.00
Basic Fuchsin	126	544	Ethanol	438.00
Basic Fuchsin	129	549	Ethanol	438.00
Basic Red 29	131	511	Water	514.00
Basic Yellow 11	132	395	Methanol	421.00
Bathophenathrolinedisulfonic Acid	133	276	Water	245.00
Benzopurpurin 4B	135	500	Water	219.00
Biebrich Scarlet, water soluble	137	505	Methanol	313.00
3,3-(4,4-Biphenylene)Bis(2,5-Diphenyl-2H-Tetrazolium)	139	250	Methanol	358.00
Bis-N-Methylacridinium Nitrate	141	430	Methanol	272.00
Bismarck Brown R	142	468	Ethanol	352.00
Bismarck Brown Y	144	457	50% ethanol & 5ml 1N Hcl	347.00
Blue Tetrazolium	146	253	Methanol	271.00
Bordeaux R	148	518	Water	219.00
Brilliant Black BN	150	570	Water	399.00
Brilliant Blue G	151	610	Ethanol	477.00
Brilliant Blue R	153	585	Ethanol	194.00
Brilliant Cresyl Blue ALD	155	622	50% Ethanol	526.00
Brilliant Crocein MOO	158	510	Water	403.00
Brilliant Green	160	625	50% Ethanol	366.00
Brilliant Sulphaflavine	162	422	Water	197.00
Brilliant Yellow	164	497	0.1N NaOH	396.00
Bromochlorophenol Blue, water soluble	166	590	Water	340.00
Bromocresol Green	168	423	Methanol	215.00
Bromocresol Green, water soluble	170	617	Water	326.00
Bromocresol Purple	171	419	Methanol	210.00
Bromocresol Purple, water soluble	173	585	0.1N NaOH	348.00
Bromophenol Blue	174	598	0.005N NaOH in Methanol	194.00
Bromophenol Blue, water soluble	176	589	Water	341.00
2-(5-Bromo-2-Pyridylazo)-5-(Diethylamino)Phenol	177	443	Methanol	338.00
Bromopyrogallol Red	178	552	Water	359.00
Bromothymol Blue	180	420	Methanol	335.00

Dye	#	EXP Abs. (nm)	Solvent	Computed Abs. (nm)
Bromoxylenol Blue	183	417	Methanol	216.00
6-Butoxy-2,6-Diamino-3,3-Azodipyridine	185	435	Methanol	351.00
Carminic Acid	193	495	Methanol	267.00
Chicago Sky Blue 6B	198	618	Water	476.96
Chlorophenol Red	200	572	0.1N NaOH	197.65
Chlorophenol Red,water soluble	202	575	Water	235.30
Chrome Azurol S	203	429	Water	325.71
Chromotrope 2R	207	510	Methanol	243.45
Chromoxane Cyanine R	209	512	Methanol	366.62
Chrysophenine	213	389	Water	411.90
Cibacron Brilliant Yellow 3G-P	217	404	Water	308.64
Congo Red	220	497	Water + 1ml 1% Na2CO3	401.32
o-Cresolphthalein	226	566	0.1N NaOH	202.66
o-Cresolphthalein Complexone	228	575	0.1N NaOH	200.13
m-Cresol Purple, sodium salt	231	436	Water	202.43
Cresol Red, water soluble	234	425	Ethanol	334.97
Cresyl Violet perchlorate	237	602	Ethanol	539.46
Crocein Orange G	238	482	Water	393.69
Darrow Red	242	502	50% Ethanol	521.00
4,6-Diamidino-2-Phenylindole dihydrochloride hydrate	244	349	Water	334.00
3,6-Diaminoacridine hemisulfate	245	456	Methanol	275.00
3,6-Diaminoacridine hydrochloride	247	456	Methanol	275.00
Diazo Red RC	248	372	Water	198.00
4,5-Dibromofluorescein	249	450	Methanol + 1 drop 1 N HCL	393.00
2,7-Dichlorofluorecein	251	509	Ethanol + 1 drop 1 N NaOH	224.00
5,7-Dichloro-8-Hyroxyquinoline	253	253	Chloroform	239.00
2,6-Dichloroindophenol, sodium salt hydrate	255	605	Water + 2ml 1N NaOH	485.00
1,1Diethyk-4,4-Carbocyanine Iodide	256	703	Methanol	576.00
Diiodofluorescein	257	522	Methanol	387.00
4-(Dimethylamino)Benzaldehyde	259	250	10% HCl	276.00
5-(4-Dimethylaminobenzylidene) Rhodanine	261	451	Methanol	342.00
4-Dimethylamino-2-Methylazobenzene	263	???	???????	325.00
4,7-Diphenyl-1,10-Phenanthroline	265	288	Chloroform	245.00
Direct Black 22	267	481	Water	380.00
Direct Blue 71	268	594	Water	409.00
Direct Orange 31	269	428	Water	365.00
Direct Red 23	270	507	Water	509.00
Direct Red 75	272	522	Water	522.00
Direct Red 81	274	508	Water	369.00

Dye	#	EXP Abs. (nm)	Solvent	Computed Abs. (nm)
Direct Violet 51	276	549	Water	350.00
Direct Yellow 8	277	390	Water	387.00
Direct Yellow 27	278	393	Water	360.00
Direct Yellow 29	279	402	Water	391.00
Direct Yellow 50	280	390	Water	219.00
Direct Yellow 62	281	341	Water	232.00
Disperse Blue 1	282	620	50% Ethanol + 1 drop 1N NaOH	231.00
Disperse Blue 3	284	640	50% Ethanol	236.00
Disperse Blue 14	285	640	50% Ethanol	237.00
Disperse Orange 1	286	483	50% Ethanol	534.00
Disperse Orange 3	287	443	50% Ethanol	533.00
Disperse Orange 13	288	426	50% Ethanol	377.00
Disperse Orange 25	289	455	Methanol	536.00
Disperse Red 1	290	503	50% Ethanol	533.00
Disperse Red 13	291	517	50% Ethanol	550.00
Disperse Red 19	292	495	50% Ethanol	446.00
Disperse Yellow 3	293	357	50% Ethanol	326.00
Disperse Yellow 5	294	405	50% Ethanol	608.00
Disperse Yellow 7	295	388	50% Ethanol	339.00
Disperse Yellow 9	296	359	Chloroform	658.00
Emodin	298	521	0.1N NaOH	257.00
Eosin B	300	514	Water + 2ml 1% sodium cardon	354.00
Eosin B, spirit soluble	302	522	Methanol	427.00
Eosin Y	304	514	Water + 1 ml 1% sodium carbor	473.00
Eosin Y, free acid	306	521	Water + 1 ml 1% sodium carbor	396.00
Eosin Y lactone	307	524	Methanol	226.00
Eriochrome Blue Black 2B	310	528	Water + 1ml 1N HCl	397.00
Eriochrome Red B	311	483	Methanol	404.00
Erioglaucine	312	625	Water	447.29
Erythrosin B	314	525	Water + 1 ml 1% sodium carbor	483.00
Erythrosin B, spirit soluble	316	533	Methanol	401.00
Ethidium Bromide	318	525	Methanol	225.00
Ethyl Eosin	320	532	Ethanol	458.00
Ethyl Orange, sodium salt	322	472	Water	321.00
Ethyl Red	324	447	0.1N NaOH	321.00
Ethyl Violet	325	596	Water	272.00
Evans Blue	327	611	Water	471.00
Fast Black K salt	329	457	Water	241.66
Fast Blue B salt	332	371	Water	202.12

Dye	#	EXP Abs. (nm)	Solvent	Computed Abs. (nm)
Fast Blue BB base	334	318	Ethanol	213.72
Fast Blue BB salt	336	395	Water	400.31
Fast Blue RR	337	319	Methanol	213.66
Fast Garnet GBC base	342	328	50 % Ethanol + 1ml 1N HCl	198.08
Fast Garnet GBC salt	344	360	Water	437.87
Fast Green FCF	345	624	50% Ethanol	452.33
Fast Red ITR base	351	256	Dioxane	215.04
Fast Red ITR salt	352	357	Water	190.09
Fast Red PDC salt	353	352	Methanol	233.79
Fast Red TR salt	354	285	Water	204.17
Fast Red Violet LB base	355	293	Methanol	204.11
Fast Red Violet LB salt	356	342	Water	380.64
Fast Violet B	358	297	Ethanol	211.56
Fast Yellow	360	480	0.1N HCl	325.57
Fast Yellow GC salt	362	324	Water	201.13
Fat Brown RR	366	451	Ethanol	354.52
Flavazin L	369	407	Water	356.68
Flavianic Acid hydrate	370	428	Water	204.29
Fluorescein	373	496	0.1N NaOH	432.39
Fluorescein, water soluble	375	491	Water	474.85
Fluoresein Diacetate	376	490	Ethanol	194.41
Fluorescein Isothiocyanate, isomer I	377	490	0.1 NaOH	457.81
Fluoresceinamine, isomer I	379	496	Ethanol + 1ml 0.1N NaOH	386.90
Fluoresceinamine, isomer II	381	495	0.1N NaOH	386.78
Fluorescent Brightener 28	382	350	Methanol	338.13
Gallocyanine	386	620	Ethanol	485.67
Guinea Green B	390	618	Water	300.44
Haba	392	348	1% phosphate buffer, pH 6.2	192.96
Hematoxylin	394	292	Methanol	219.35
Hoechst 33258	396	343	Methanol	337.55
3-Hydroxy-4-(2-Hydroxy-4-sulfo-1-Naphthylazo)-2NCA	398	570	Methanol	443.51
7-Hydroxy-4-Methylcoumarin	399	322	Methanol	231.87
Hydroxy Naphthol Blue, disodium salt	401	650	Methanol + 10ml Water	418.46
8-Hydroxyquinoline-5-sulfonic acid monhydrate	402	315	Methanol	241.24
Indigo	403	602	Chloroform	233.00
Indigo Carmine	405	608	Water	198.00
Indocyanine Green	407	775	Water	472.00
Indoine Blue	409	598	Methanol	538.00

Dye	#	EXP Abs. (nm)	Solvent	Computed Abs. (nm)
Janus Green B	411	660	50% ethanol	514.00
Lacmoid	415	611	Metahnol	415.00
Leuco Crystal Violet	418	261	0.1N HCl in Methanol	250.00
Leucomalachite Green	419	262	Chloroform	193.00
Light Green SF Yellowish	421	630	Water	194.00
Lissamine Green B	423	633	Water	247.00
Lucifer Yellow VS	429	427	Water	257.00
Lumichrome	430	392	Methanol	229.00
Luxol Brilliant Green BL	432	624	Methanol	479.00
Malachite Green Carbinol hydrochloride	437	615	Water	196.10
Martius Yellow monohydrate	440	432	Methanol	454.39
Metanil Yellow	446	414	Methanol	312.45
Methylene Blue	448	661	Water	486.80
Methylene Violet Bernthsen	453	580	50% ethanol + 10ml 0.1N HCl	412.12
Methylene Violet 3RAX	455	557	Water	291.87
Methyl Eosin	456	520	Water	492.50
Methyl Green, zinc chloride salt	458	629	Water	517.86
Methyl Orange	461	507	Water + .5ml 1N HCl	324.78
Methyl Red	464	410	Methanol	324.16
Methyl Red hydrochloride	466	493	Methanol + 1ml 1N HCl	313.10
Methyl Red, sodium salt	467	437	Methanol	494.11
Methyl Yellow	472	408	Methanol	323.71
Mordant Blue 9	473	516	Water + 1ml 1N HCl	197.69
Mordant Brown 1	474	373	Water	378.43
Mordant Brown 4	475	500	Ethanol	380.93
Mordant Brown 6	476	400	Water	193.02
Mordant Brown 24	477	400	Water	336.04
Mordant Brown 33	478	442	Water	384.91
Mordant Brown 48	479	492	Water	360.12
Mordant Orange 1	480	385	Methanol	326.44
Mordant Orange 6	482	381	Water	352.80
Mordant Orange 10	483	386	Water	353.83
Mordant Red 19	484	413	Water	364.38
Mordant Yellow 7	485	365	Methanol	326.51
Mordant Yellow 10	486	354	Methanol	324.17
Mordant Yellow 12	487	380	Water	346.21
MTT-Methylthiazolyldiphenyl Tetrazolium	488	378	Methanol	271.14
Naphthochrome Green	490	362	Water	226.32
Naphthol AS	491	394	1N NaOH	234.49

Dye	#	EXP Abs. (nm)	Solvent	Computed Abs. (nm)
Naphthol Blue Black	496	618	Water	462.72
Naphthol Yellow S	500	428	Water	442.15
a-Naphthyl Red	503	439	Methanol	360.96
Neutral Red	504	540	50% ethanol + .5 acetic acid	491.41
New Coccine	506	506	Water	236.32
New Fuchsin	508	533	50% ethanol	428.74
Nile Blue chloride	518	638	50% Ethanol	572.09
Nile Red	519	553	Methanol	360.57
Nitrazine Yellow	521	586	0.1N NaOH	457.42
Nitro Red	527	572	Water	451.89
2-Nitroso-1-Naphthol	528	262	Chloroform	226.21
1-Nitroso-2-Naphthol-3,6-Disulfonic Acid, disodium	530	424	0.1N NaOH	225.50
Nuclear Fast Red	532	535	Water	248.21
Oil Blue N	534	637	Ethanol	236.68
Oil Red EGN	536	521	Chloroform	382.17
Oil Red O	537	518	Toluene	386.32
Orange G	539	475	Water	371.84
Orange II	541	483	Water	363.80
Palatine Chrome Black 6BN	545	569	Water	426.45
Palatine Fast Yellow BLN	548	440	Water	190.60
Para Red	549	488	Toluene	366.07
Pararosaniline acetate	551	545	50% ethanol	276.23
Pararosaniline base	552	544	Ethanol	190.82
Phenanthrenequinone	555	270	Chloroform	251.76
1,10-Phenanthroline	557	264	Methanol	236.67
1,10-Phenanthroline monohydrate	559	264	Ethanol	236.59
1,10-Phenanthroline monohydrochloride monohydrate	560	264	Methanol	236.64
Phenazine Methosulfate	561	386	Water	262.59
Phenolphthalein	563	552	Water + 2ml 1N NaOH	192.47
Phenol Red	565	557	Water + 20ml boric buffer, pH 9	195.48
Phenol Red, water soluble	567	423	Methanol	328.40
4-Phenylazoaniline	568	386	Methanol	193.97
4-Phenylazoaniline hydrochloride	570	385	Methanol	193.89
4-Diphenylamine	571	411	Ethanol	322.56
4-phenylazomaleinanil	572	329	Chloroform	262.59
4-Phenylazophenol	574	347	Methanol	193.21
9-Phenyl-2,3,7-Trihydroxy-6-Flouorone	576	552	0.1N NaOH	396.37
Philoxine B	577	548	50% ethanol	424.05
Pinacyanol chloride	579	604	Ethanol	567.93

Dye	#	EXP Abs. (nm)	Solvent	Computed Abs. (nm)
Plasmocorinth B	581	527	Water	252.30
Ponceau S	583	520	Water	388.95
Ponceau SS	585	514	Water	452.55
Potassium Indigotrisulfonate	586	600	Water	199.49
Primulin	588	356	Water	371.21
Purpurin	592	485	Methanol	236.76
4-(2-Pyridylazo)Resorcinol, monosodium salt hydrate	594	411	Methanol	444.01
Pyrocatechol Violet	596	441	Methanol	345.17
Pyrogallol Red	597	480	Ethanol	417.40
Pyronin Y	601	548	50% Ethanol	485.06
Quinalizarin	604	512	Methanol	434.71
Quinizarin	606	250	Chloroform	212.04
Quinoline Yellow A, spirit soluble	608	413	Methanol	221.02
Reactive Black 5	611	597	Water	416.83
Reactive Blue 2	612	607	Water	298.41
Reactive Blue 4	614	595	Water	239.57
Reactive Red 8	617	500	Water	301.33
Remazol Brilliant Blue R	620	592	Water	430.87
Resorufin	625	573	Methanol	552.31
Rhodamine 123 dihyrate	626	501	Water	424.00
Rhodamine B	628	543	Methanol	461.53
Rhodamine B base	630	544	Methanol	238.39
Rhodamine 6G	631	524	Water	448.69
Rhodamine 6G perchlorate	633	528	Methanol	207.44
Rhodamine 6G tetrafluoroborate	634	528	Methanol	451.26
Rose Bengal	637	548	Water + 1ml 1% sodium carbon	495.32
Rosolic Acid	640	482	Ethanol + 2ml 1N HCl	345.46
Safranin O (Y,T)	645	530	50% ethanol	240.00
Solvent Blue 35	647	652	Chloroform	237.00
Solvent Blue 59	648	642	Ethanol	237.00
Solvent Green 3	649	644	Acetone	235.00
Stains-All	651	575	Ethanol	238.00
Sudan I	653	476	Ethanol	369.00
Sudan II	654	493	Methanol	372.00
Sudan III	656	507	Toluene	383.00
Sudan IV	658	520	Toluene	369.00
Sudan Black B	660	598	Ethanol	404.00
Sudan Orange G	662	400	Methanol	322.00
Sudan Red 7B	664	533	Toluene	307.00

Dye	#	EXP Abs. (nm)	Solvent	Computed Abs. (nm)
Sulfobromophthalein sodium hydrate	666	577	0.1N NaOH	199.00
Sulfonazo III, tetrasodium salt	667	567	Water	295.00
2-(4-Sulfophenylazo)-1,8-Dihydroxy-3,6-Naphthalenedisulfonic acid	669	507	Water	238.00
Sulforhodamine 101 hydrate	671	576	Ethanol	439.00
Sulforhodamine 101 acid chloride	672	578	Ethanol	438.00
sulforhodamine B	674	554	0.1N NaOH in methanol	231.00
Sulforhodamine G	676	529	Methanol	235.00
Tartrazine	678	425	Water	346.14
Tetrabromophenol Blue	680	610	50% ethanol + 5 ml pH 5.0 buffe	195.61
Tetrabromophenol Blue, water soluble	682	610	Water	338.54
3,3,5,5-Tetrabromophenolphthalein	683	310	0.01N NaOH	195.36
Tetrabromophenolphthalein Ethyl Ester, potassium salt	684	593	Methanol	456.94
3,4,5,6-Tetrabromophenolsulfonephthalein	685	426	Methanol	323.53
4,5,6,7-Tetrachlorofluorescein	686	518	Methanol	390.34
3,3,5,5-Tetraiodophenolphthalein	689	315	0.1N NaOH	205.50
3,3,5,5-Tetraiodophenolsulfonephthalein	692	433	Methanol	352.32
3,3,5,5-Tetramethylbenzidine dihydrochlorid hydate	695	288	Methanol	216.28
Thiazol Yellow G	698	402	Water	351.94
Thioflavin T	701	412	Water	439.69
Thionin	703	598	Water	534.14
Thymol Blue	706	594	0.1N NaOH	341.66
Thymolphthalein	709	592	0.1N NaOH	204.20
Thymolphthalein Monophosphoric Acid	711	445	0.1N NaOH	207.84
Tiron	712	291	Water	209.53
Toluidine Blue O	714	626	Water	548.99
Toluidine Red	716	507	Toluene	193.95
Tropaeolin O	719	490	0.1N NaOH	329.52
Trypan Blue	721	607	Methanol	220.29
Uniblue A, sodium salt	724	596	Water	413.62
Variamine Blue Rt salt	725	377	Water	437.24
Victoria Blue B	727	599	Ethanol	443.59
Victoria Blue R	729	615	Methanol	441.23
Victoria Pure Blue BO	730	619	Water	457.32
Violamine R	732	529	Water	266.84
Xylenol Blue	737	424	Methanol	202.00
Xylenol Blue,water soluble	739	425	Methanol	334.00
Xylenol Orange,water soluble	740	580	0.1N NaOH	333.00
Xylidine Ponceau 3RS	742	503	Water	234.00
Xylidyl Blue I, water soluble	744	612	Ethanol + 2ml 0.08M borax buff	384.00

Dye	#	EXP Abs. (nm)	Solvent	Computed Abs. (nm)
Zincon	745	490	0.1N NaOH	375.00
Zincon, monosodium salt	747	490	Methanol	375.00